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Rotating Anisotropies Without Superparamagnetic Grains in Exchange Bias Systems

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ABSTRACT

We introduce a random field model with anisotropic interfacial exchange for ferromagnet / antiferromagnet bilayers and calculate average coupling energies and coupling directions for different grain or domain sizes. The model is shown to reconcile Malozemoff's random field Ising model for exchange bias with the spinflop coupling mechanism. Furthermore, we find that for small and mid size domains, the average coupling direction strongly varies between different interfacial configurations. We show how this behavior can lead to rotating anisotropies in systems with very strong magnetocrystalline anisotropies, where the use of superparamagnetic grains or domains in the antiferrofmagnet is not justified.

INTRODUCTION

The most frequently discussed effects in ferromagnetic (FM) / antiferromagnet (AFM) bilayers is the shift in the magnetization curve that can be observed when the system has been cooled in an external field[1]. The magnitude of the shift is inversely proportional to the thickness of the FM layer which implies that the effect is directly related to the interfacial exchange between the FM and AFM and the effect is thus referred to as *exchange anisotropy* or *exchange bias* [2, 3]. The temperature below which the exchange bias is observed is called blocking temperature (T_B), it is typically equal or somewhat smaller than the Neel temperature (T_N) of the AFM. It is commonly believed that the bias sets in when the AFM spins order and a sufficient number of domains in the AFM are blocked such that the AFM spins do not reverse when the FM magnetization is inverted during the measurement of the magnetization curve.

In most cases, hysteretic effects such as a strong increase in coercivity are observed along with the onset of exchange bias[4-6]. Most models to explain these effects are based on an idea of Fulcommer and Charap [7], where, assuming that the FM couples in some form to the AFM, magnetic structure of smaller grains or domains in the AFM will be dragged along irreversibly with the FM magnetization and lead to hysteresis, while the larger grains, in which the magnetic order is locked in, will lead to the bias effect. Stiles and McMichael [8] introduced the notion of a *rotating anisotropy* which follows the FM magnetization when the external field is rotated and is attributed to magnetically "loose" grains in the AFM. With this model they were able to explain a direction independent shift in the resonance field of ferromagnetic resonance experiments.

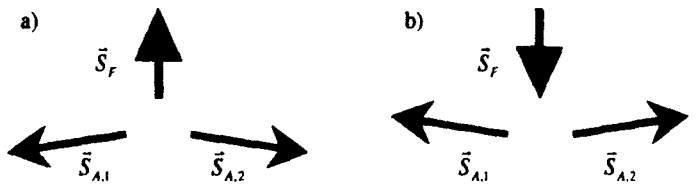

Figure 1: Model of three spins where the F-A part of the exchange energy is given by $E_{exch}^{F-A} = -\sum_{i=1,2} J_i \vec{S}_F \cdot \vec{S}_{A,i} + \sum_{i=1,2} \vec{D}_i \cdot (\vec{S}_F \times \vec{S}_{A,i})$.

While the concept of a superparamagnetic structure in smaller grains or domains in the AFM is reasonable for systems with weak magnetocrystalline anisotropy such as NiO, it is not clear why is should apply to an AFM like CoO where the anisotropy energy is of the same order as the exchange energy[9]. In the present contribution we show that within the random field model a variable effective coupling direction that arises from adjustment of the walls in smaller and mid-sized AFM domains will lead to a rotating anisotropy. In this picture most AFM moments are frozen and dissipative effects are due to irreversible motion of domain walls.

RANDOM FIELD MODEL WITH ANISOTROPIC EXCHANGE

In order to understand how the net coupling direction of the FM to an AFM domain can vary without rotating the AFM domains, we first have to investigate the microscopic coupling mechanisms between the AFM and the FM moment. For interfaces with compensated exchange between the FM and the AFM, i.e. where the FM spins couple equally to all AFM sublattices[10], the following two models are typically discussed in the literature[11, 12]:

1. The random field model [13-15], in which the AFM is assumed to break up into domains. The finite area of these domains will result in a net interfacial exchange which scales as $\left(1/\sqrt{N}\right)$ if N is the number of AFM-FM pairs. In this model the FM and AFM spins are assumed to be collinear which leads to a change in exchange energy $\Delta E = 2J/\sqrt{N}$ when the FM spins are reversed. The random field model is commonly used to explain the net unidirectional coupling between the FM and individual AFM domains (or grains).
2. The spin-flop coupling model [16, 17], which assumes Heisenberg spins and where the frustrated exchange across the interface leads to a slight canting to the AFM moments and a net coupling of the FM that is perpendicular to the AFM easy axis. In contrast to the random field Ising model the coupling is uniaxial and does not lead to exchange bias [18, 19]. Furthermore, the coupling strength is independent of the AFM domain / grain size.

The collinearity required by the random field Ising model is only justified for small domains in the AFM. For most realistic domain/grain sizes, the spin-flop mechanisms will dominate [8] leaving the origin of the unidirectional coupling as a puzzle. We will now show that spin-flop coupling can have a unidirectional component when the

anisotropic Dzyaloshinsky-Moriya (DM) term is added to the exchange, i.e. the exchange energy between two moments on sites i and j has the form

$$E_{ij} = -J_{ij}\vec{s}_i\vec{s}_j + \vec{D}_{ij}\left(\vec{s}_i \times \vec{s}_j\right). \qquad (1)$$

In cases where the crystal structure has a center of inversion at the point bisecting the line between i and j, $\vec{D}_{ij}$ can be shown to vanish [20, 21]. While this symmetry condition holds in most bulk system, it is never satisfied at the AFM/FM interface[22] and the DM term thus has to be included to properly describe interfacial exchange. The consequence of the DM term is that the difference in exchange energy upon reversal of the FM spins is different from zero in the spin-flop coupling state. This is best illustrate by considering three spins (see Figure 1), $\vec{S}_F$, $\vec{S}_{A,1}$, and $\vec{S}_{A,2}$, in the spin-flop coupling states. The energy difference when $\vec{S}_F$ is reversed (Figures 1a and 1b) is $\Delta E_{xchg} = 2\left(D_{1,z} + D_{2,z}\right)$.

In order to estimate the magnitude of the unidirectional term in the case of a FM/AFM bilayer, we perform a calculation using the random field model with anisotropic interfacial exchange. We consider a bilayer with bcc type lattice and a (110) interface with nearest neighbor exchange J in the FM and $-J$ in the AFM. In the AFM we further assume uniaxial anisotropy along the (001) direction with K/J=1. For the interfacial exchange we use Eq. (1) with $J_{ij} = Jr$ and $D_{ij} = Dr'\left(\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta\right)$, where $r \in [-1,1]$, $r' \in [-1,1]$, $\vartheta \in [0,\pi)$, and $\varphi \in [0,2\pi)$ are uniform random variables. These random fluctuations are usually justified with the large variation of the interfacial bond lengths that results from the large lattice mismatch between the FM and AFM in systems like CoO/Permally or FeF2/Fe. The particular system we consider here consists of 5 layers in the AFM and 10 layers in the FM. We use periodic boundary conditions parallel to the interface with variable unit cell

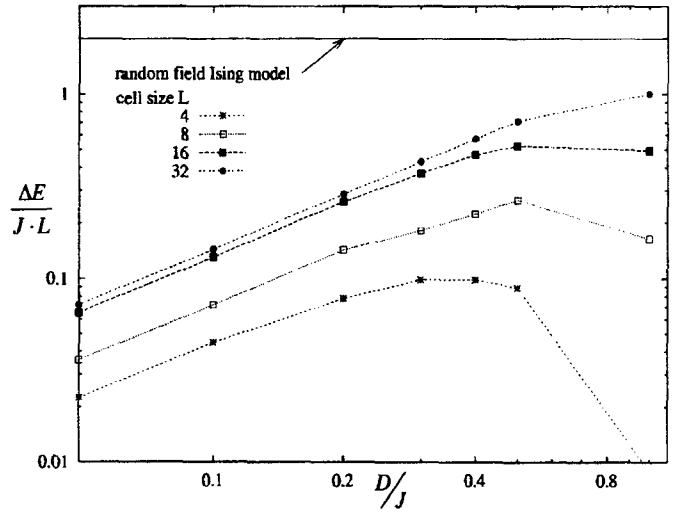

Figure 2: Energy change due to reversal of the FM spins for AFM-FM bilayers (see text for details) for Heisenberg spins with random anisotropic interfacial exchange and different sizes of the computational cell (symbols) compared to expected result from the random field Ising model (solid line)

size consisting of L by L primitive cells (L = 2, 4, 8, 16, and 32). The effect of the magnetostatic interaction is treated as an effective hard axis in the FM perpendicular to the interface. We seek to calculate AFM/FM coupling energies as a function of domain size, where we equate the unit cell size of our model to the domains size. For this we have to suppress the formation of further domains within the unit cell. We have therefore prepared an ordered AFM spin configuration and randomized FM spins as an initial condition and subsequently minimized the energy using the Landau Lifshitz equations (see [19] for details). When the energy minimum is reached, the FM spins are inverted and the energy is again minimized. For all but the smallest unit cells this procedure always yields two distinct states. Their energy differences, averaged over 40 random configurations, are plotted in Figure 2 and compared to the result of the random field Ising model. While the unidirectional anisotropy due to the DM term is systematically smaller than that of the random field Ising model, it has nevertheless comparable order or magnitude provided D/J is not too small. Moria [21] estimated $D/J \sim 0.1$ in bulk AFM but values that are as large as 0.5 have been reported for systems with lower symmetry [23].

EFFECTIVE COUPLING DIRECTION AND ROTATING ANISOTROPIES

In the previous section we have determined energy differences averaged over many random configurations of the interfacial exchange interactions. The direction of the FM magnetization with regard to the AFM easy axis for each of these configurations is plotted in Figure 3. By choosing appropriate initial conditions for the minimization procedure discussed above, the system can always be prepared in a way that the global

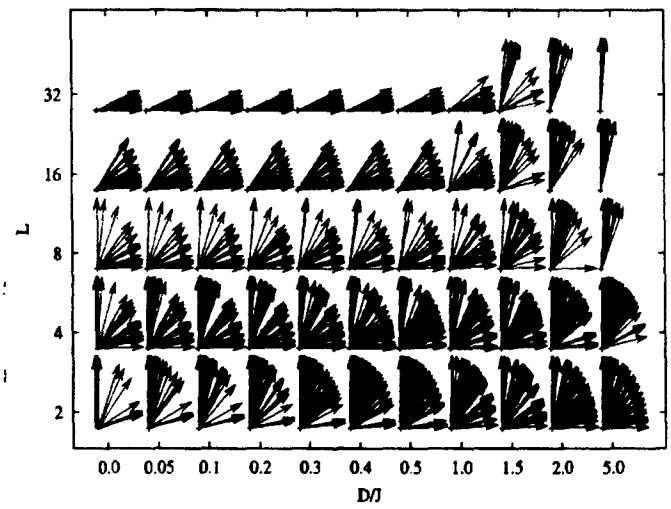

Figure 3: Average direction of FM spins for every random configuration. The AFM easy axis, (001), is taken to be parallel to the y-axis of the plot. In the case D=0 and L=2 (4), 80% (50%) of the configurations are collinear with the AFM easy axis.

energy minimum has the FM moments pointing at angle between 0 and 90 degrees with regard to the AFM easy axis (this choice of initial condition corresponds to the field cooling procedure). As expected, the coupling is always collinear for small cells and perpendicular when the cells are large. When the anisotropic exchange is non zero, the coupling direction strongly varies between different configurations of the smaller and mid size cell but is always perpendicular to the AFM easy axis when the cells are large.

As was done in the previous section, we consider the cell size in the model to correspond to domain sizes in the film and further recognize that different domains correspond to different random configurations of the interfacial exchange in the computational cell. To simplify the argument, let us assume that the field was applied along the (1-10) direction during the field cooling procedures, i.e. perpendicular to the AFM easy axis. The domain pattern in the AFM will arrange itself such that the coupling direction of most domains is parallel to the cooling field. When the direction of the applied field and the FM magnetization is subsequently rotated to a different direction, the AFM domain pattern will adjust by moving domain walls to minimize the energy. While it remains to be shown explicitly, the displacement of such domain walls in real samples, with defects at which these walls are pinned, is likely an irreversible process. According to the results plotted in Figure 3, the coupling direction of the larger domains will not be affected by the rearrangement of domain walls. Together with the energy differences plotted in Figure 2, this will lead to a unidirectional anisotropy that has similar order of magnitude as that found with the random field Ising model. Since the coupling direction of the smaller domains depends strongly on the random configuration, changing the domain pattern will lead to new configuration with adjusted coupling directions that follows the FM magnetization. This will give rise to a rotating component of the anisotropy which adjusts with direction of the applied field. In this model the dissipation would take place in the irreversible displacement of domain walls in the AFM and thus does not require the superparamagnetic rotation of all the moments in smaller grains.

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